TECHNISCHE UNIVERSITÄT DARMSTADT

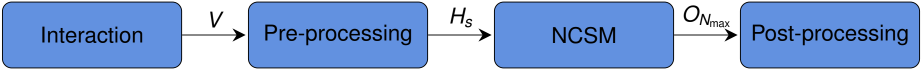
From Chiral Interactions to NCSM Observables

Tobias Wolfgruber

SFB 1245

SFB 1245 Workshop 2022

No-Core Shell Model Toolchain



Chiral EFT Interactions

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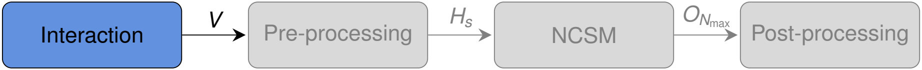

- NN+3N order-by-order interactions from chiral EFT
  - based on QCD symmetries with nucleons and pions as active DoF
  - systematically improvable
  - order-by-order allows for robust uncertainty estimates
- two main interactions currently in use
  - nonlocal NN interaction developed by Entem, Machleidt, Nosyk with corresponding 3N interaction Hüther *et al.* PLB 808, 135651 (2020)
  - semilocal momentum-space regularized NN+3N interaction developed within the LENPIC collaboration Maris *et al.* PRC 103, 054001 (2021)

Comparison: Nonlocal and Semilocal Interaction

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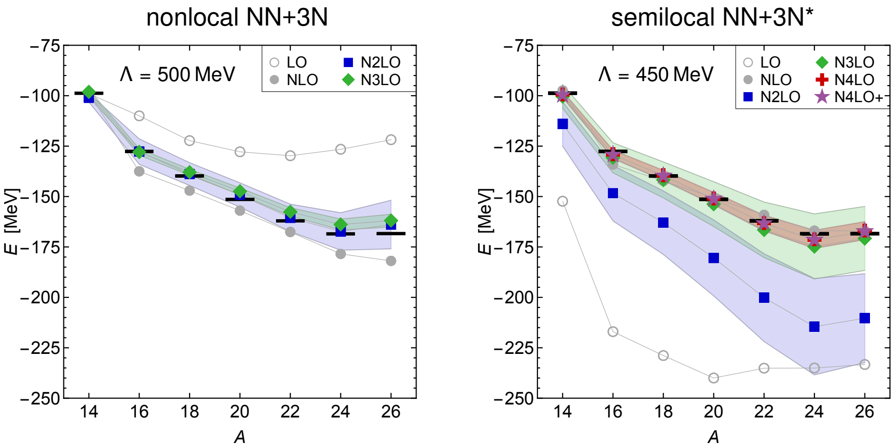
nonlocal EMN

- nonlocal regularization (both long and short-range contributions)
- 3N low-energy constants (LECs) fitted to a mix of few- and many-body observables
- currently available at orders
  NN: up to N^4LO
  3N: up to N^3LO

semilocal LENPIC

- locally regularized long-range interaction (unmodified pion physics)
- nonlocal regularization of short-range interaction
- 3N LECs fitted solely in few-body space
- currently available at orders
  NN: up to N^4LO+
  3N: up to N^2LO

Ground-State Energy for the Oxygen Chain



Point-Proton Radius for the Oxygen Chain

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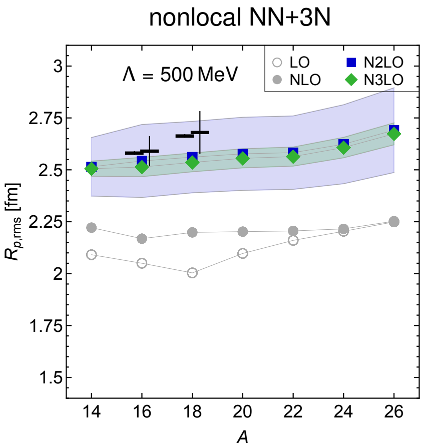
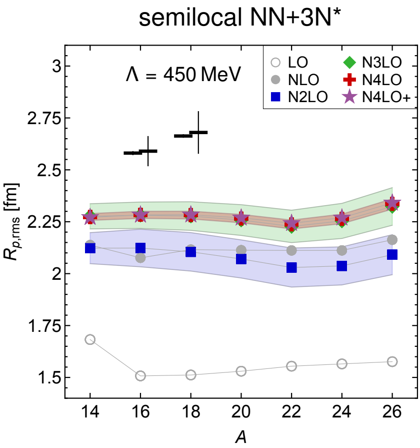
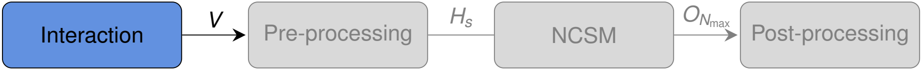




Current Status of Interactions



- both interactions show good results for ground-state energies
- significant underprediction of radii with current iteration of LENPIC interaction
  - feature of semilocal regularization scheme
  - expect improvements with
    – 2-body corrections to the charge radius operator
    – the inclusion of 3N interaction at N^3LO

Post-Processing NCSM results with Neural Networks

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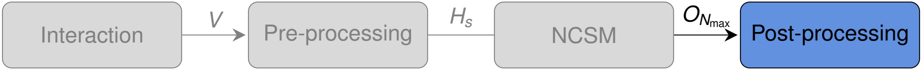

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- significant underprediction of radii with current iteration of LENPIC interaction
  - feature of semilocal regularization scheme
  - expect improvements with
    - 2-body corrections to the charge radius operator
    - the inclusion of 3N interaction at N^3LO
- application of artificial neural networks (ANN) to extract converged results from NCSM calculations
  - precise predictions of ground-state energies and radii
  - more stable and consistent results than classical methods
  - robust uncertainty estimates

No-Core Shell Model

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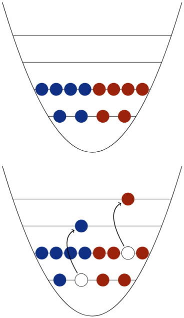
- stationary Schrödinger equation as matrix eigenvalue problem

$$\sum_j \langle \phi_i | H | \phi_j \rangle \langle \phi_j | \psi_n \rangle = E_n \langle \phi_i | \psi_n \rangle \quad \forall i,$$

- 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



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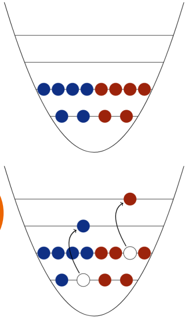
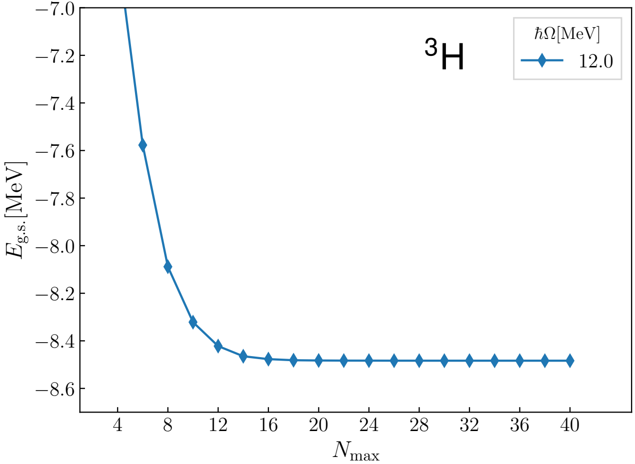
  - dependency on HO frequency $\hbar\Omega$
- truncate model space by number of excitation quanta N_{max} w.r.t. the lowest-energy Slater determinant
- **convergence controlled by two parameters**

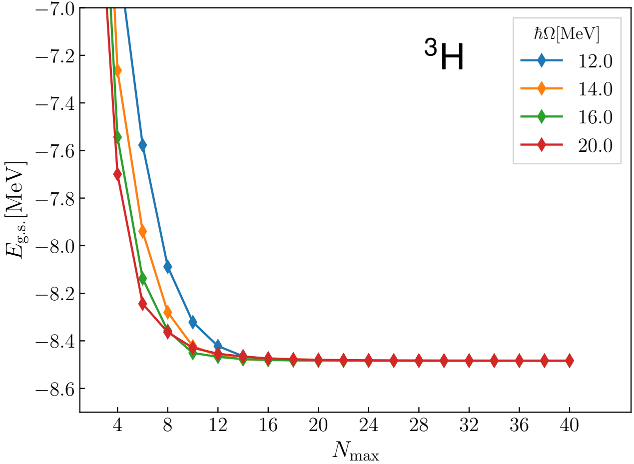


Convergence Behavior



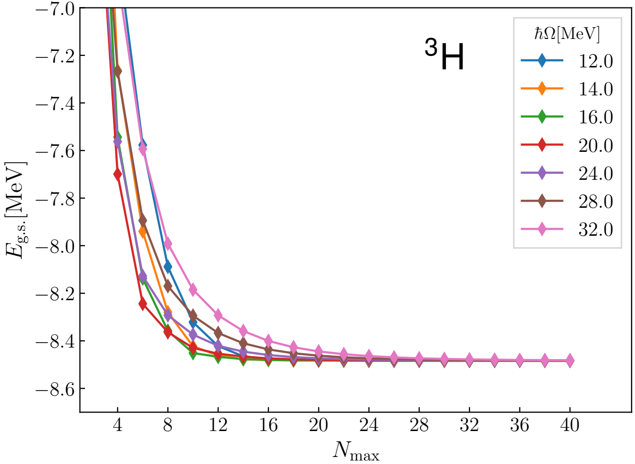
- monotonously decreasing with N_{max}

Convergence Behavior



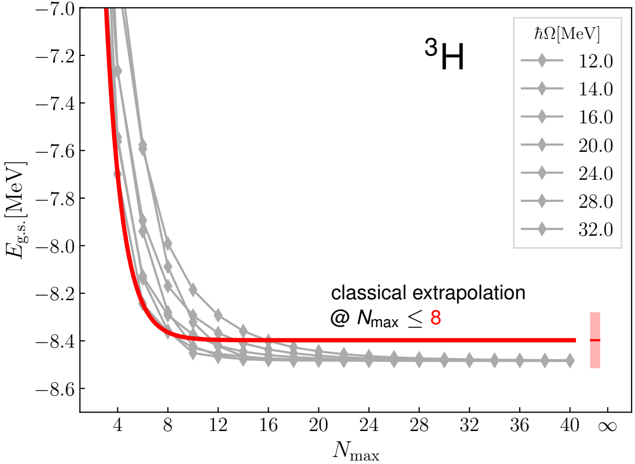
- monotonously decreasing with N_{max}
- different rates of convergence for different HO frequencies

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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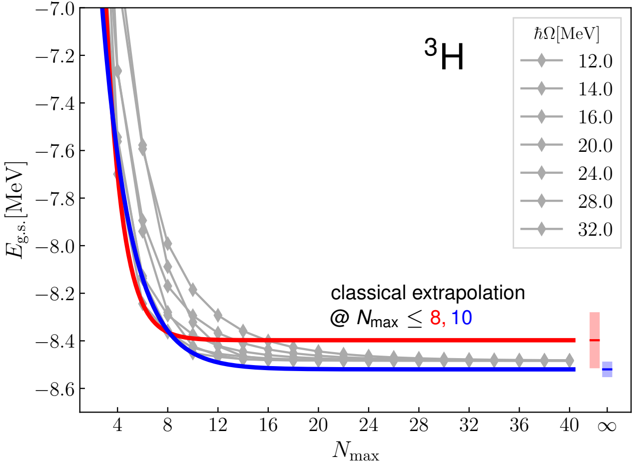

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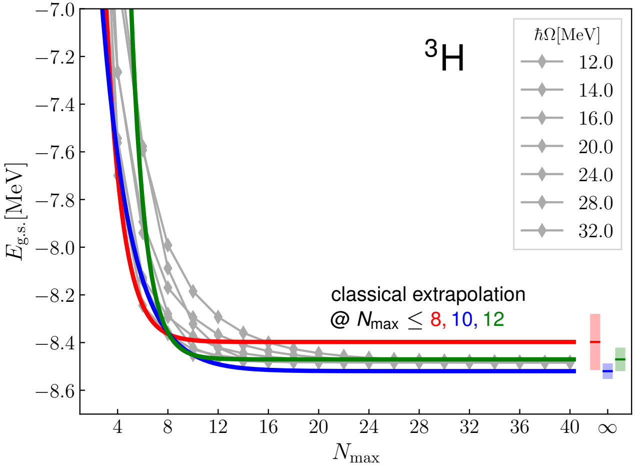
Convergence Behavior

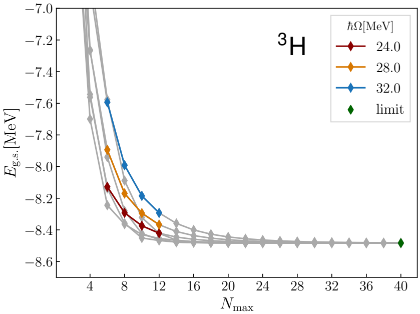


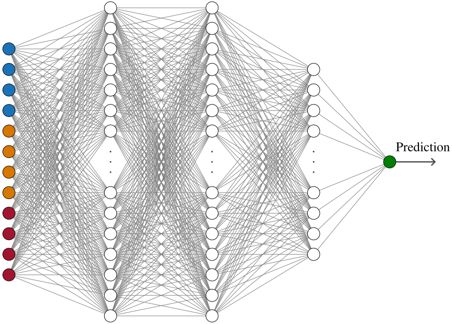
- monotonously decreasing with N_{max}
- different rates of convergence for different HO frequencies
- all sequences share the same limit

Machine Learning Approach

- previous applications: capture $f(N_{\text{max}}, \hbar\Omega)$
- 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)





ANN Input Modes

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ABS

- feed in raw energy values $E_{\hbar\Omega}^{N_{max}}$ for 4 consecutive N_{max}
- target: E^{∞}
- may struggle with large output range
- requires random scaling/shifting to prevent biases

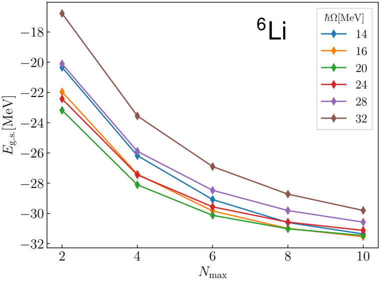
DIFF

- feed in the differences of 4 consecutive energy values: $\Delta_{\hbar\Omega}^{N_{max}} = E_{\hbar\Omega}^{N_{max}} - E_{\hbar\Omega}^{N_{max}-2}$
- target: $\Delta^{\infty} = E^{\infty} - \min(E_{\hbar\Omega_i}^{\mathcal{N}_{max}})$
- reduce output range/scale dependence

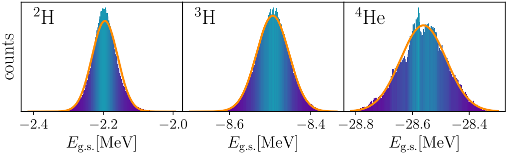
MINMAX

- like ABS, but normalize sample to interval [0, 1]
- target: scaled accordingly
- normalize every input sample individually
- alleviates scale dependence

Statistical Evaluation

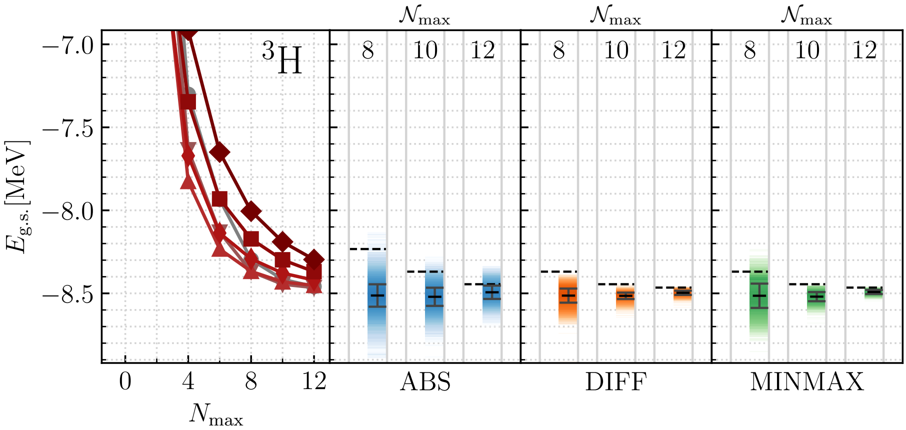


- different family of interactions
  Maris et al. PR C 103, 054001 (2021)
- construction of evaluation samples analogoulsy to training samples
- different predictions from one ANN
- turn to statistical approach



- apply 1000 ANN
- prediction and uncertainty from Gaussian fit

Application to Few-Body Systems



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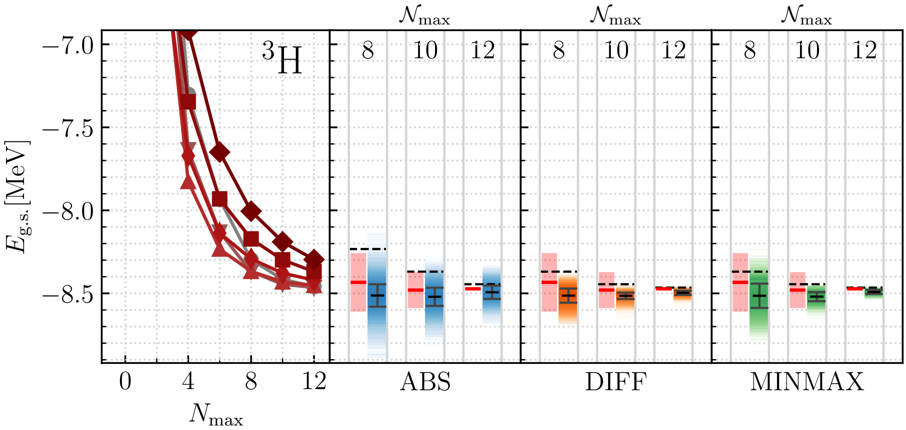

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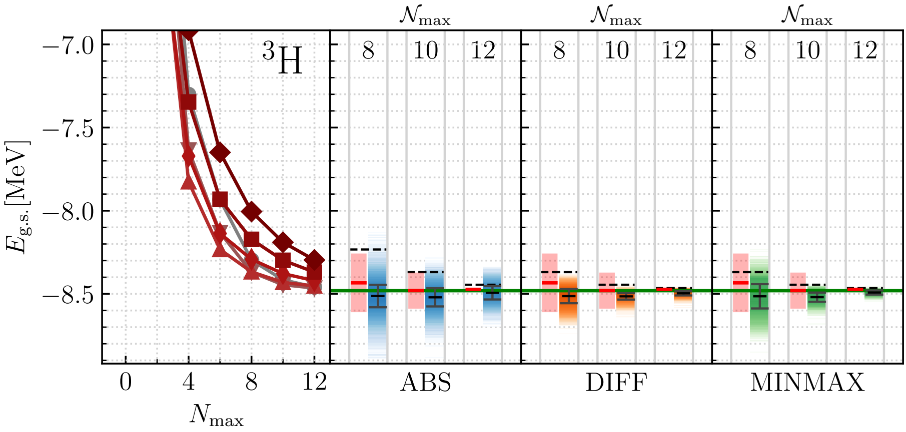
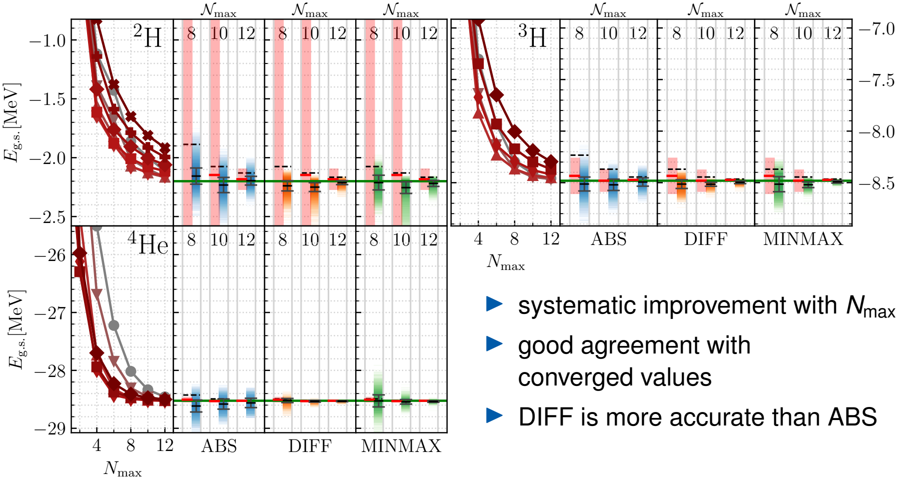
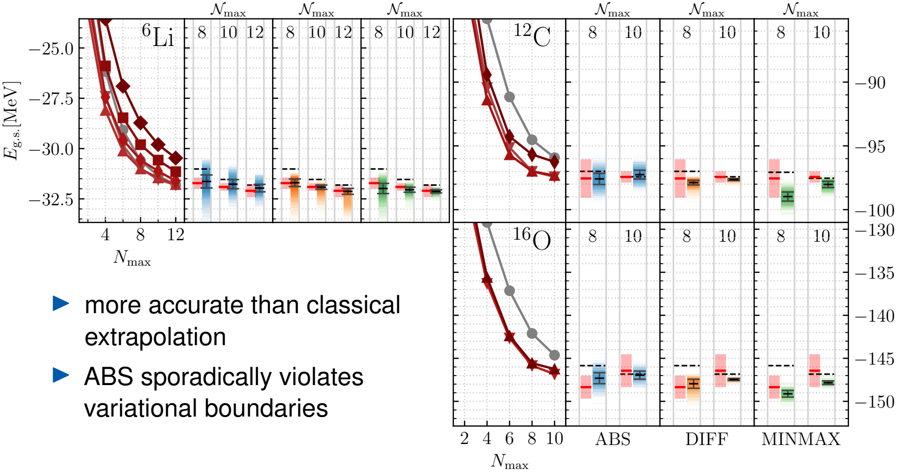


Application to Few-Body Systems



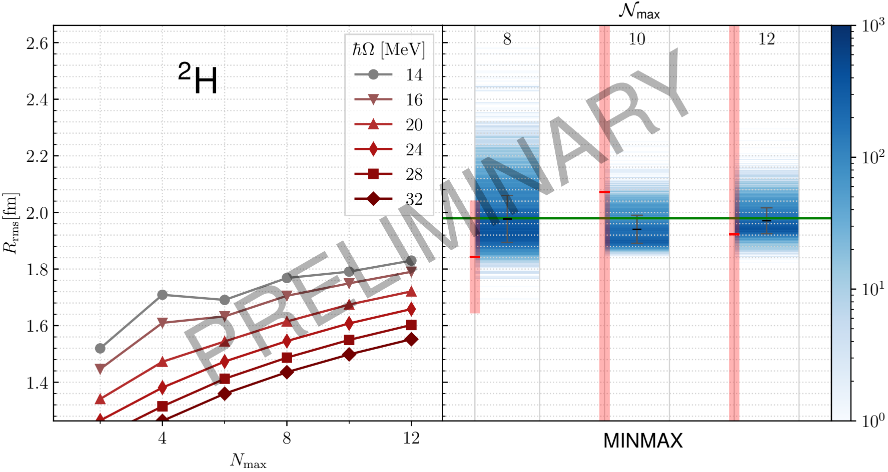
- systematic improvement with $N_{\max}$
- good agreement with converged values
- DIFF is more accurate than ABS

Application Beyond Few-Body Systems



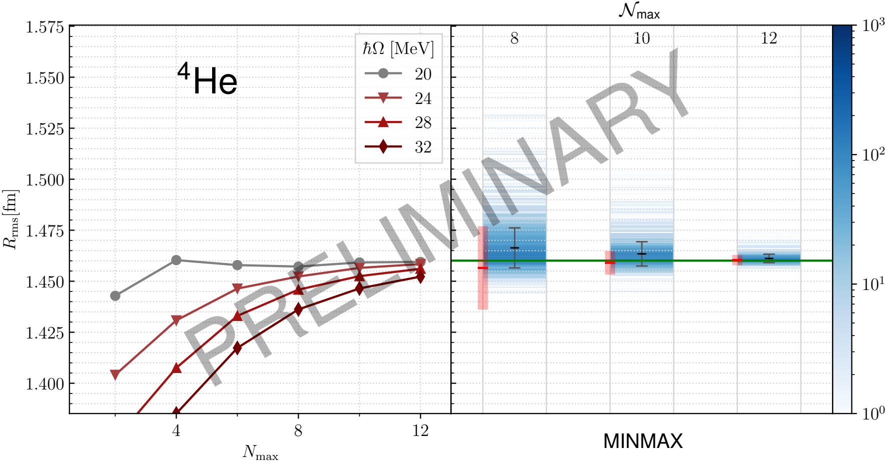
- more accurate than classical extrapolation
- ABS sporadically violates variational boundaries

Radii – ^{2}H



$\mathcal{N}_{\max}$
8
10
12
^{2}H
$\hbar\Omega$ [MeV]
14
16
20
24
28
32
R_{rms}[fm]
2.6
2.4
2.2
2.0
1.8
1.6
1.4
4
8
12
$N_{\max}$
10^3
10^2
10^1
10^0
PRELIMINARY
MINMAX

Radii – ^{4}He



4He
ħΩ [MeV]
20
24
28
32
R_rms [fm]
1.575
1.550
1.525
1.500
1.475
1.450
1.425
1.400
4
8
12
N_max
𝒩max
8
10
12
MINMAX
10^3
10^2
10^1
10^0
PRELIMINARY

Conclusion & Outlook

- ANNs provide robust predictions with reliable uncertainty estimates
  - more accurate than classical extrapolations
  - robust w.r.t. changes in the training data
- applicable to any nucleus accessible via NCSM
- extension to radii (work in progress) and other observables
  - challenge: more complex convergence patterns
- great potential for optimization:
  - normalization of training data
  - adjustment of topology and hyperparameters
- Knöll, TW, Agel, Wenz, Roth: arXiv:2207.03828

Thank you for your attention!

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- **thanks to my group and collaborators**

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C. Wenz, N. Zimmermann

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computing time

Hessisches Kompetenzzentrum für Hochleistungsrechnen

DFG