Towards a Machine Learning description of Nuclei

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Advances in Many-Body Theories: From First Principle Methods to Quantum Computing and Machine Learning - November 2$^{\mathrm{nd}}$ - 6$^{\mathrm{th}}$ 2020

Keeble, J. W. T., and A. Rios. "Machine learning the deuteron." PLB 809 (2020): 135743. / arxiv (2019): 1911.13092

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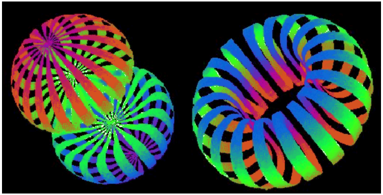
- Proof of principle calculation
- Deuteron chosen as **benchmark** to compare with numerical results.
- Used Entem-Machleidt Interactions N3LO *PRC **68**, 041001 (2003)*
- Separate centre of mass with relative motion (effective one-body problem)
- Solved in momentum-space to avoid expensive Laplacian calculation



Shapes of the deuteron in the lab. reference frame. Stripes show surfaces of equal density for $M_j = 1$ (left) and $M_j = 0$ (right). Courtesy of http://www.phy.anl.gov/theory/movie-run.html.

PYTORCH

Benefits of using PyTorch

- Scalability of Neural Networks
- Direct calculation of gradients via Autograd
- Portability to multiple GPUs
- Dynamic Computational Graph

Deuteron	N^3LO
$B_d(MeV)$	2.224575
$r_d(fm)$	1.978
$Q(fm^2)$	0.285
$P_D(\%)$	4.51

*PRC **68**, 041001 (2003)*

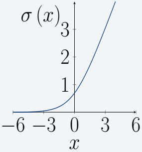
Neural Network Ansatz

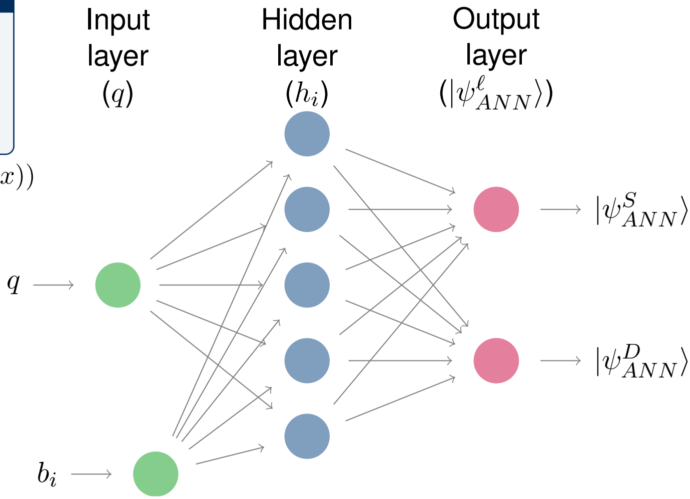
Weight Init.

- $\mathcal{W}^{(1)} \in [-1, 0)$
- $b^{(1)} \in [-1, 1)$
- $\mathcal{W}^{(2)} \in [0, 1)$

$$\sigma(x) = \ln(1 + \exp(x))$$

Activation function





1 $\text{N}_{hid} \equiv 4$ weights

$$h_i = \sigma\left(\mathcal{W}_i^{(1)} q + b_i^{(1)}\right) \qquad |\psi^{\ell}_{ANN}\rangle = \sum_i^{N_{hid}} \mathcal{W}_{i\ell}^{(2)} h_i$$

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Energy training - Ground-state

Energy Minimisation

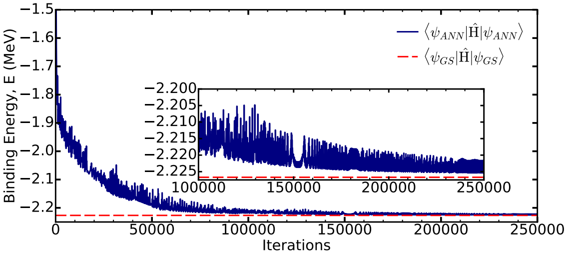
$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \to \frac{\partial E}{\partial \mathcal{W}} = \frac{2}{\langle \Psi | \Psi \rangle} \left(\langle \frac{\partial \Psi}{\partial \mathcal{W}} | \hat{H} | \Psi \rangle - E \langle \frac{\partial \Psi}{\partial \mathcal{W}} | \Psi \rangle \right)$$

RMSprop

$$\nu_t = \beta_2 \nu_{t-1} + (1 - \beta_2) \left(\frac{\partial E}{\partial \mathcal{W}_t} \right)^2$$

$$\mathcal{W}_{t+1} = \mathcal{W}_t - \frac{\alpha}{\sqrt{\nu_t} + \epsilon} \frac{\partial E}{\partial \mathcal{W}_t}$$

G. Hinton, Uni. Toronto, CSC321, (2012)



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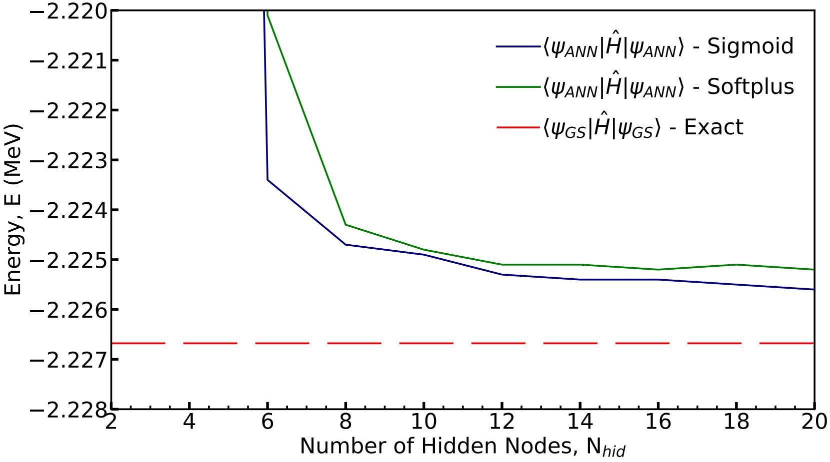
Energy



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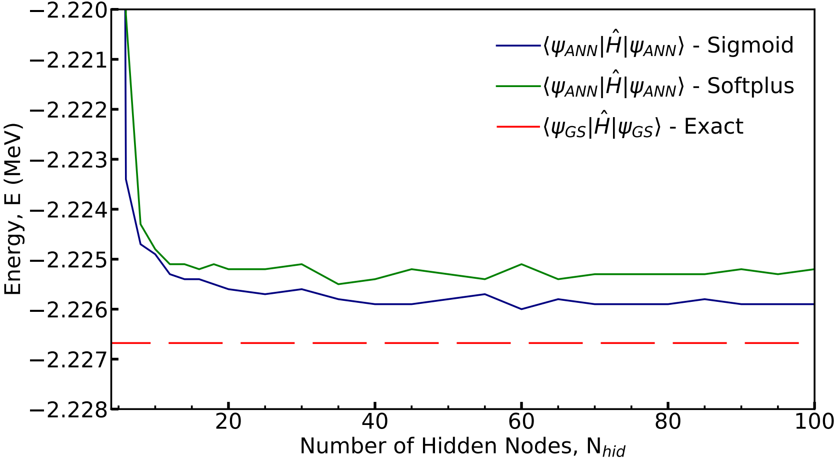

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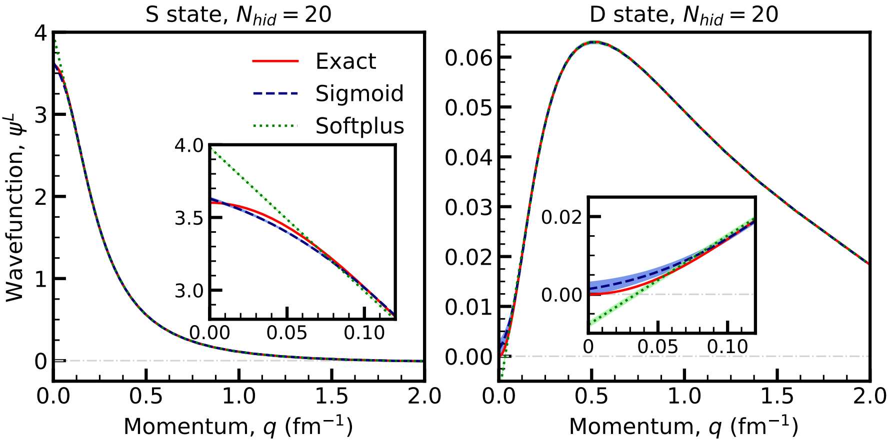
Wavefunction Reconstruction



$$\langle\Psi|\hat{H}|\Psi\rangle = 4\pi \int_0^\infty \int_0^\infty q^2 \Psi \hat{H} q'^2 \Psi \, dq \, dq' \approx 4\pi \sum_{i,j} w_i q_i^2 \Psi_i \hat{H}_{ij} w_j q_j'^2 \Psi_j$$

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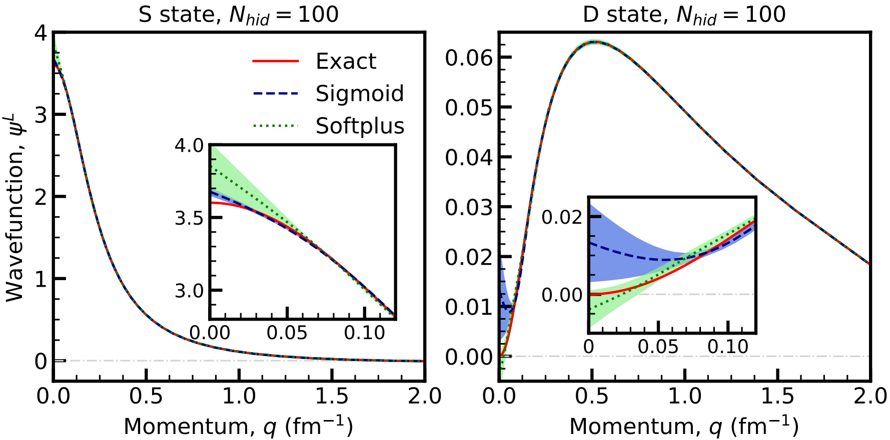

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How can we model larger systems?

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Deuteron

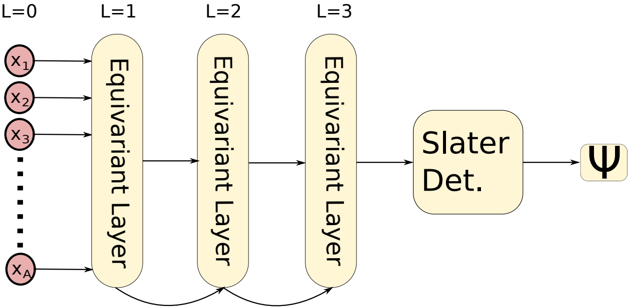
- We have demonstrated that vANNs **can solve** nuclear problems
- **Agreement with benchmark** to within **0.1%** and constant variance
- Bias-Variance tradeoff pushed towards **zero cost** regions

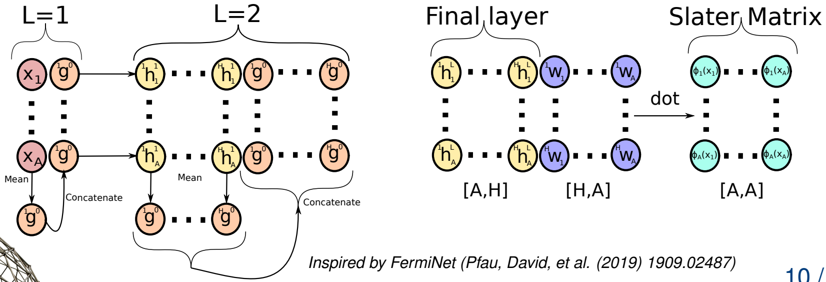
Challenges ahead

There are 3 main challenges that variational artificial neural networks need to overcome in order to solve a nuclear system

- Nuclear interaction ✓
- Antisymmetrisation of vANNs ✓
- Implementing spin degrees of freedom **?**

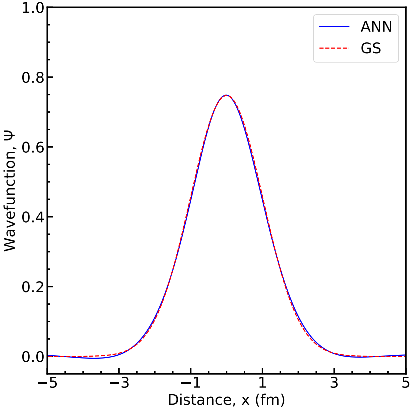
Antisymmetric Ansatz

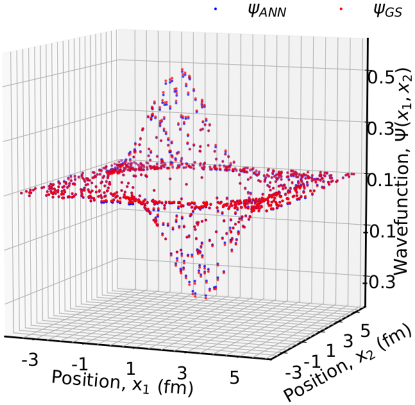




Inspired by FermiNet (Pfau, David, et al. (2019) 1909.02487)

The 1D Harmonic Oscillator





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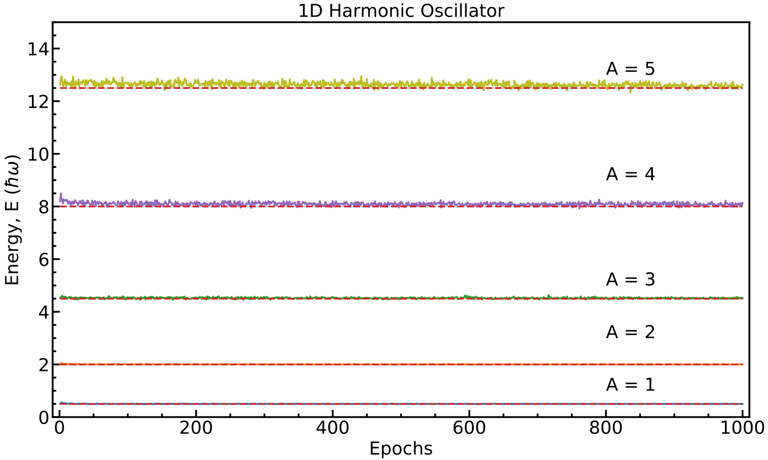

Concluding remarks

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Deuteron

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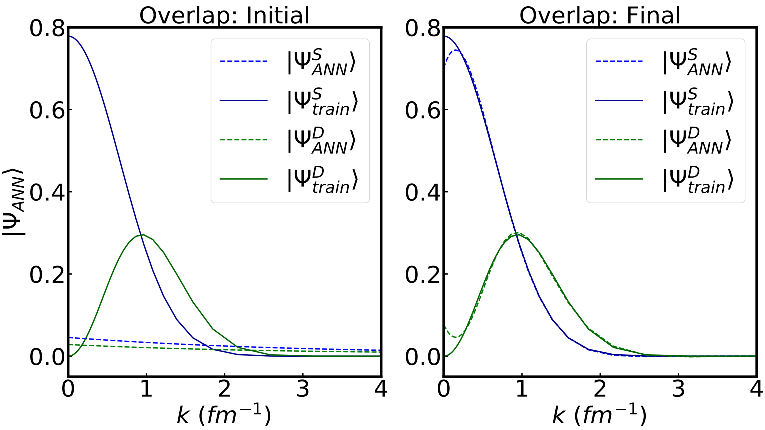
Many thanks to: Arnau Rios, Mehdi Drissi,
Pierre Arthuis, Paul Stevenson

Science & Technology Facilities Council

Backup slides...

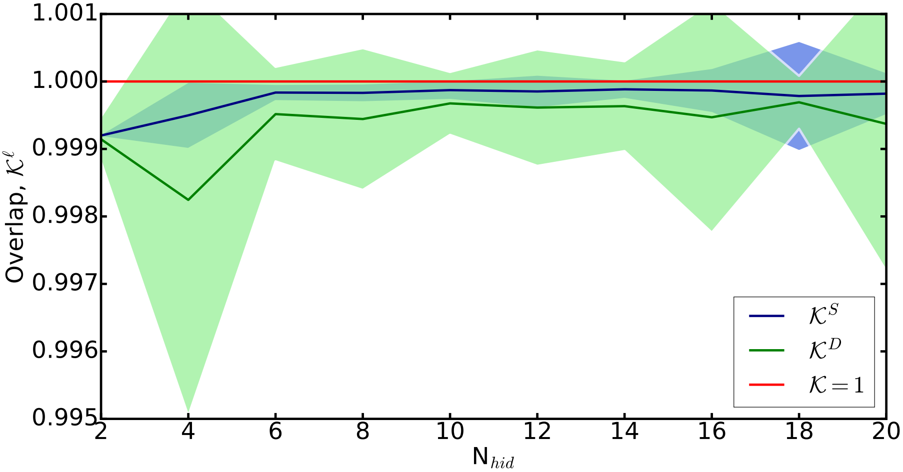
Pre-training - Before and After



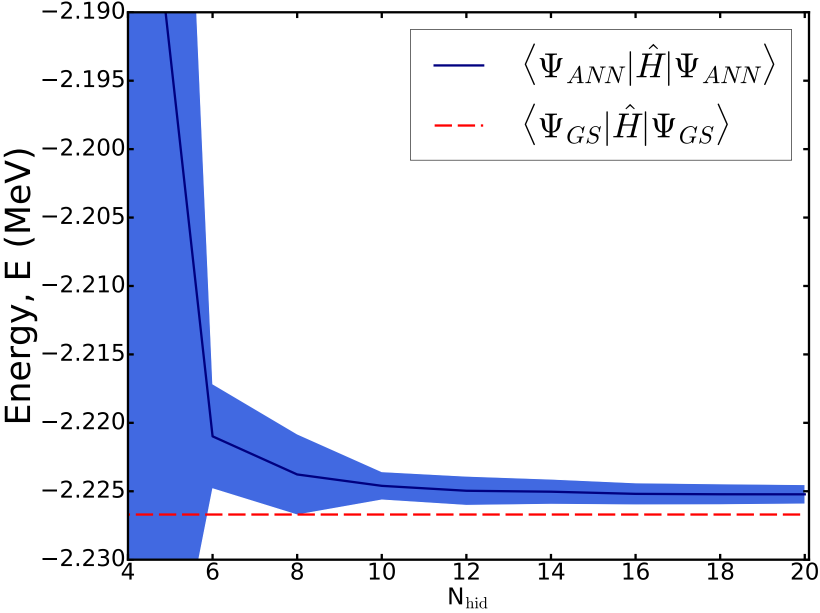
$$\mathcal{K}^{\ell} = \frac{\langle \psi^{\ell}_{train} | \psi^{\ell}_{ANN} \rangle^2}{\langle \psi^{\ell}_{train} | \psi^{\ell}_{train} \rangle \langle \psi^{\ell}_{ANN} | \psi^{\ell}_{ANN} \rangle}$$

$$|\psi^{\ell}_{train}\rangle = \mathcal{A}^{\ell} k^{\ell} \exp\left(-0.5 b^2 k^2\right)$$

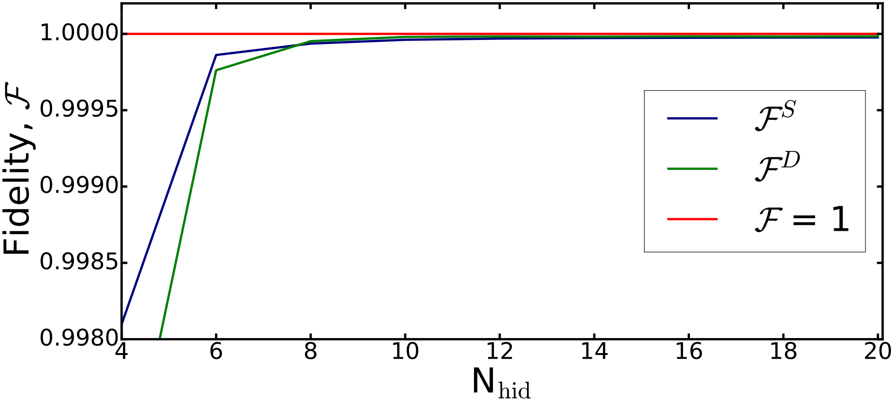
Pre-training - Results



Energy training - Results

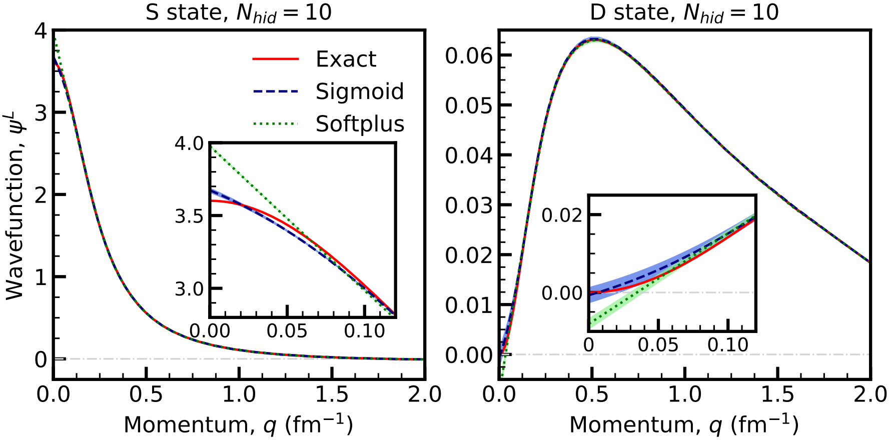


Wavefunction Reconstruction - Fidelity

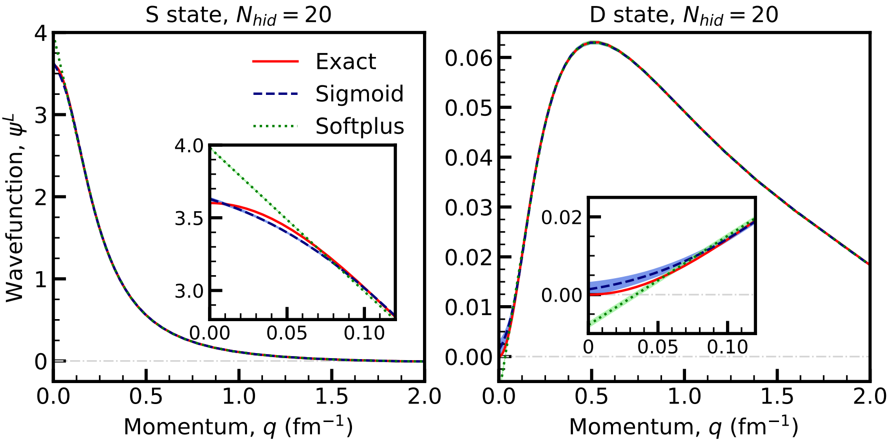


$$\mathcal{F}^{\ell} = \frac{\langle \psi^{\ell}_{g.s.} | \psi^{\ell}_{ANN} \rangle^2}{\langle \psi^{\ell}_{g.s.} | \psi^{\ell}_{g.s.} \rangle \langle \psi^{\ell}_{ANN} | \psi^{\ell}_{ANN} \rangle}$$

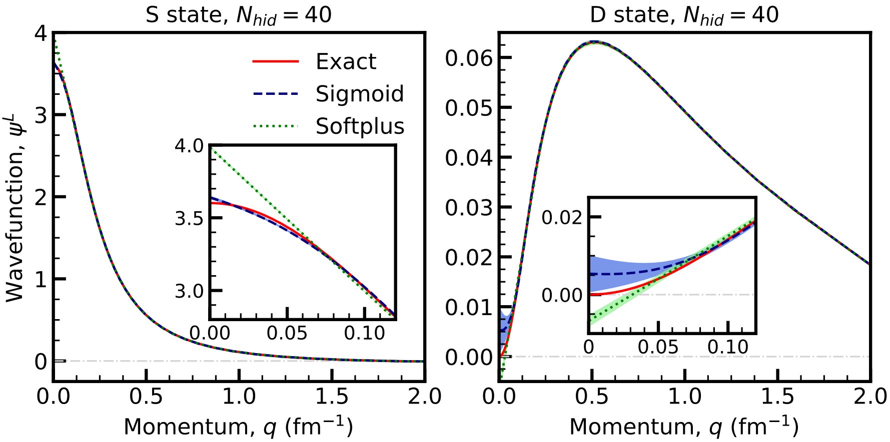
Bias-Variance trade-off: N_{hid} = 10



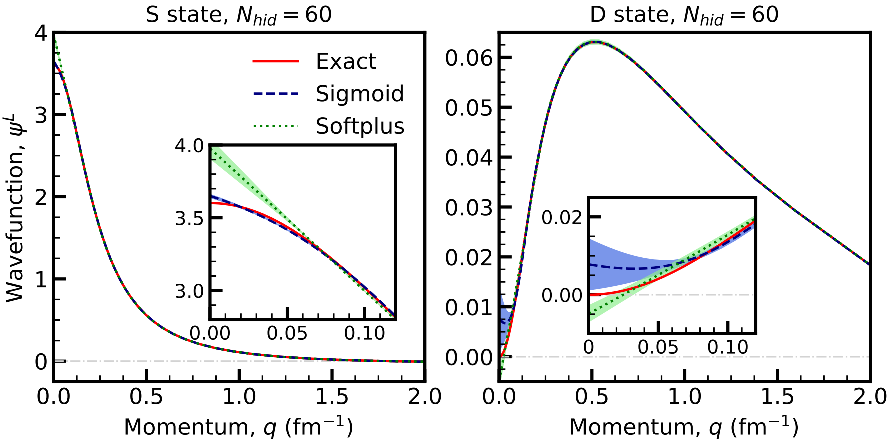
Bias-Variance trade-off: N_{hid} = 20



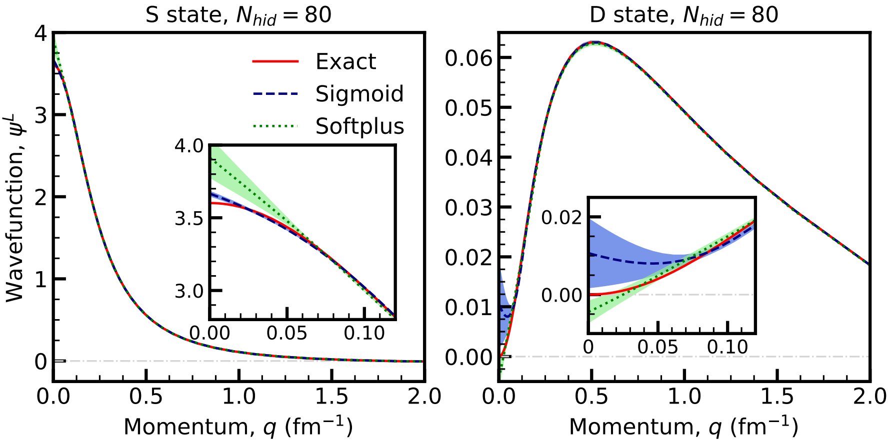
Bias-Variance trade-off: N_{hid} = 40



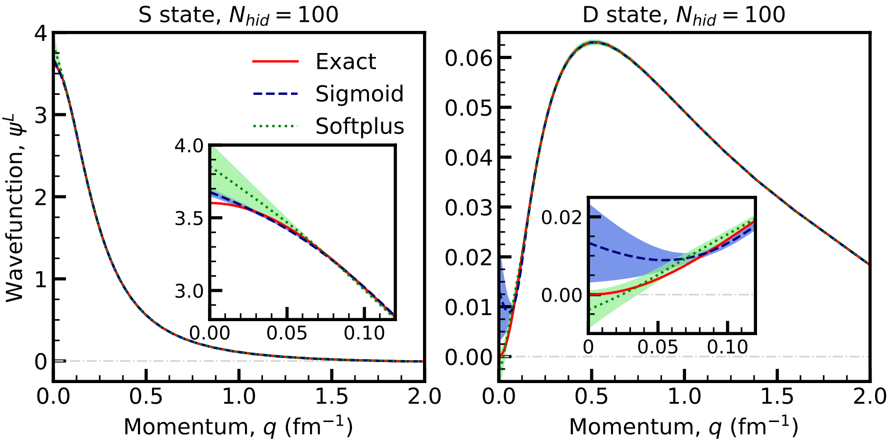
Bias-Variance trade-off: N_{hid} = 60



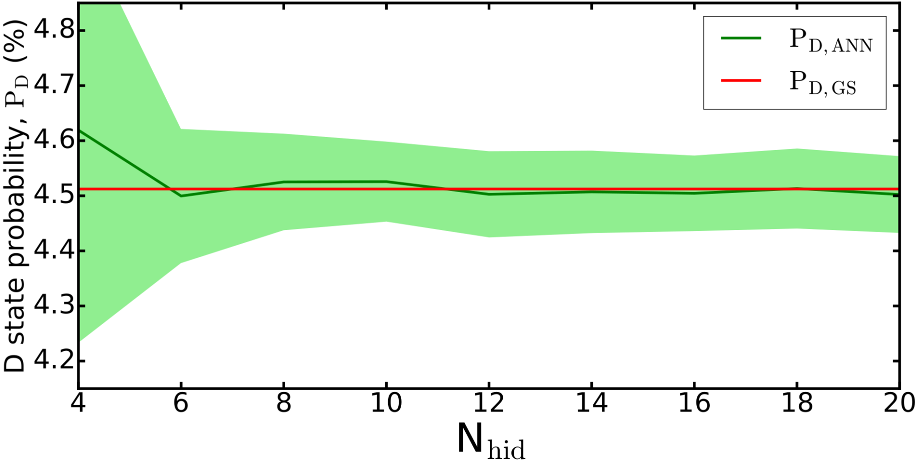
Bias-Variance trade-off: N_{hid} = 80



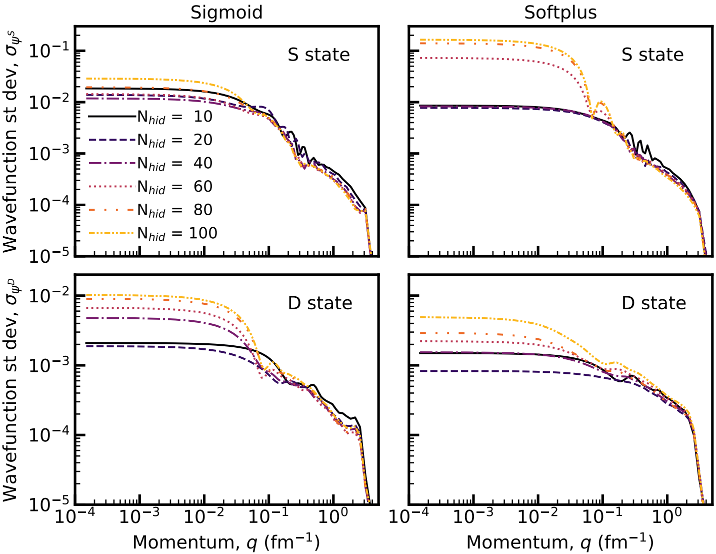
Bias-Variance trade-off: N_{hid} = 100



D-state Probability



Bias-Variance Tradeoff



Potential Energy Error Analysis

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